

Chemistry 209

Introductory Spectroscopy & Structure

Lectures in B1-271: 11:30-12:20 MWF. Tutorial in AL-113, 2:30 Friday

Course Instructor: Professor Robert J. Le Roy

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Office Hours: MW 2:30-5:30 and F 3:30-5:00 (unless otherwise posted)

This course will introduce you to the broad field of molecular spectroscopy. In modern science, spectroscopy has become the most important probe of molecular structure, and one of the most important analytical techniques. The use of nuclear magnetic resonance spectroscopy has become central to organic chemistry and biochemistry, and the use of laser spectroscopy has revolutionized analytical and physical chemistry and chemical physics. Because of the fact that spectroscopy has become vital to most areas of chemistry and so widely used on all areas of science and scientific research, it is important for you to learn something about its principles and applications early in your scientific career. To date, we are the only University in Canada to present a course of this type at this stage in a science program.

As is becoming increasingly common at Waterloo, this course will be managed using the UW-ACE www facility at <http://uwangel.uwaterloo.ca> with which most of you are now familiar. This site will provide course information, problem set postings and solutions, schedules, supplementary lecture material, and other information that you may find useful.

The Text for the course is a comprehensive set of printed notes entitled "***A Spectroscopy Primer: An Introduction to Atomic, Rotational, Vibrational, Raman, Electronic, Photoelectron and NMR Spectroscopy***", which are available from Chemistry Stores (ESC 109; ground floor of ESC across from the year-1 lab) for \$30. We will be following these notes fairly systematically, so you are advised to read ahead, before each class, and keep track of our progress. Note that although essentially all of the course material may be found in these notes, most students have considerably greater difficulty mastering the course material if they do not also regularly attend lectures!

Glossary

A glossary of terms and symbols encountered in this course is posted on the course web site, and your ability to understand and identify these terms is one measure of your grasp of the course material. [One exam question will ask you to define or identify several of them.] You should print a copy of this page and make a point of writing out for yourself definitions/explanations of these quantities as we encounter them in the course.

Formulae Sheet

A large number of equations and formulae are presented and used in this course, and you *will not* be expected to memorize them! However, you *will be expected* to recognize them and the variables appearing therein, and to know how to use them. A copy of a standard formulae/data sheet to be provided for tests and exams is posted on the course www site. You should print a copy for yourself, and make a point of identifying and ensuring that you learn when and how to use each of the expressions listed there as we encounter them during the term.

Illness

Absences from Tests or Exams or missed problem sets may be accommodated in some manner *only if* a completed *Verification of Illness* form (available from the 'About Us' link at <http://www.healthservices.uwaterloo.ca>) is completed and turned in to the Science Undergrad Office in ESC-252. Absence for other reasons will result in a grade of **zero** for that component of the coursework.

Academic Integrity

You are expected to be familiar with UW expectations of Academic Integrity, and you are encouraged to complete the on-line quiz at <http://www.lib.uwaterloo.ca/ait/>.

Course Outline:

1. **Introduction to Spectroscopy:** (\approx 7-8 lectures)
2. **Pure Rotational, or Microwave Spectroscopy:** (\approx 5-6 lectures)
3. **Vibrational or Infrared Spectroscopy:** (\approx 5-6 lectures)
4. **Raman Spectroscopy:** (\approx 2 lectures)
5. **Electronic Spectroscopy:** (\approx 3 lectures)
6. **Photoelectron Spectroscopy:** (\approx 3 lectures)
7. **Nuclear Magnetic Resonance (NMR) Spectroscopy:** (\approx 6 lectures)

Grades:

Assignments (five or six, at roughly biweekly intervals): 10 – 15%

Midterms (two tests during the scheduled tutorial period 2:30–3:20 PM
Friday October 22 and Friday November 19), for 10 – 15% each.

Final Exam (scheduled by the Registrar during the December exam period): 55 – 70%

TOTAL: 100%

[Final weights will be determined at the end of the terms after the final exams are marked.]

NOTE: Uncollected problems set and test papers will be destroyed at the end of term.

Supplementary Material:

The Handbook of Chemistry and Physics is available both in paper format on Reserve in the Davis Centre Library (call No. QD65.H3), and electronically (<http://www.hbcnetbase.com>) from any UWaterloo IP address. Section 1, pp. 9-12, presents a table of the masses of all stable isotopes of all atoms.

The following books which have been placed on library-use reserve will provide helpful insight and alternate viewpoints on the course material.

QC 174.1.C7 *The Quantum Physicists and an Introduction to Their Physics* by William H. Cropper.
An excellent and quite readable “story book” about the history of the origins of quantum theory and the people who developed it.

QD 96.M65B36 *Fundamentals of Molecular Spectroscopy* by C.N. Banwell.
This is a somewhat more advanced text, but still useful as a reference book, and good for a more detailed look at some of the topics covered. Probably the most useful of the books on reserve.

QC 451.H65 *Modern Spectroscopy* by J.M. Hollas.
Much the same level as Banwell’s book, perhaps a bit more descriptive and modern, including a good discussion of lasers.

QD 96.M65 B76 *Molecular Spectroscopy* by J.M. Brown.
Strong emphasis on diatomic molecule spectroscopy.

QC 454.R36 F47 *Introductory Raman Spectroscopy* by J.R. Ferraro, K. Nakamoto and C.W. Brown.

QD 96.N8 A37 *NMR and Chemistry* by J.W. Akitt.
This book is a good higher-level introduction to NMR spectroscopy.

QD 96.N8 M3 *A Complete Introduction to Modern NMR Spectroscopy* by R.S. Macomber.